OPTICAL PROPERTIES OF STRAINED AND RELAXED $Si_{1-X-Y}Ge_XC_Y$

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ABSTRACT

Using spectroscopic ellipsometry we measured the pseudodielectric function of $Si_{1-x-y}Ge_xC_y$ alloys ($0 \leq x \leq 0.48$, $0 \leq y \leq 0.05$) grown on Si (001) using molecular beam epitaxy. For pseudomorphically strained layers, the energy shifts of the E_1, $E_1+\Delta_1$, E_0', and E_2 transitions are determined by line shape analysis and are due to alloy composition effects, as well as hydrostatic and shear strain. We give expressions for hydrostatic and shear shift based on continuum elasticity theory, using deformation potentials for Si and Ge, for biaxial stress parallel to the (001) growth plane in a diamond or zinc blende type crystal and applied this to the ternary Si-Ge-C alloy. The energies of E_1 and its spin orbit split partner $E_1 + \Delta_1$ agree fairly well with theory. The E_2 transitions in $Si_{1-x}Ge_x$ at around 4.3 eV depend linearly on Ge concentration. In case of relaxed layers, the E_1 and $E_1 + \Delta_1$ transitions are inhomogeneously broadened due to the influence of misfit and threading dislocations. For a silicon cap on top of a dislocated, relaxed SiGe layer, we recovered the bulk Si dielectric function.

INTRODUCTION

The binary $Si_{1-x}Ge_x$ alloy system has attracted the interest of many researchers during the past years. With recent developements and optimization of epitaxial growth techniques like molecular beam epitaxy (MBE) and chemical vapor deposition (CVD) it became possible to grow high quality strained $Si_{1-x}Ge_x$ alloys with up to 30 at. % Ge [1-4] as well as $Si_{1-y}C_y$ films [5] with carbon contents of up to 1.5%. Since Si technology is the most advanced basis for electronic devices, these compounds are promising new materials for future applications [6].

In the past, there has been some controversy about the validity of Vegard's law in binary $Si_{1-x}Ge_x$ [7-9] as well as ternary $Si_{1-x-y}Ge_xC_y$ [10] alloys. The linear approximation of the average lattice constant, i.e. Vegard's law, for a ternary bulk alloy

$$a_{xy} = (1 - x - y)a_{Si} + xa_{Ge} + ya_C \tag{1}$$

is a good approximation in most cases. For biaxially stressed layers we distinguish between the lattice constant perpendicular and parallel to the growth direction. The pseudomorphic condition $a_\perp = a_{Si}$ (growth on Si substrate) requires $a_{||} = a_{xy}(1 + e_{||})$ where $e_{||}$ is the strain parallel to [001] induced by the misfit in the plane of growth.

The optical properties of bulk strain-free $Si_{1-x}Ge_x$ alloys have been investigated by many techniques such as ellipsometry [11] and electroreflectance [12]. It was found that the best fit of E_1 and E_2 energies between the Si and Ge endpoints is given by [11, 12]

$$\begin{aligned} E_1(x) &= [3.395 - 1.287x - 0.153x(1-x)]\ \text{eV} \\ E_2(x) &= [4.372 - 0.00069(1-x)]\ \text{eV} \end{aligned} \tag{2}$$

Another group [11, 13] also reported results for $E_1 + \Delta_1$ transitions, which can only be resolved in Ge-rich alloys at room temperature.

$$(E_1 + \Delta_1)(x) = [3.428 - 1.132x - 0.062x(1-x)]\ \text{eV} \tag{3}$$

	Si[a]	Ge[b]	C[c]
E_0' (eV)	3.320	3.123	7.28
E_0' (eV)	3.319[d]	–	–
E_0' (eV)	3.300[e]	–	–
E_1 (eV)	3.396	2.111	7.48
E_1 (eV)	3.395[d]	–	–
E_1 (eV)	3.390[e]	–	–
E_2 (eV)	4.270[f]	4.368	–
	4.492[g]	–	–
c_{11} (10^{10} Pa)	16.6	12.9	–
c_{12} (10^{10} Pa)	6.4	4.8	–
D_1^1 (eV)	-9.72	-8.6	–
D_3^3 (eV)	4.36	5.9	–

Table 1: Bulk properties of Si, Ge, and C. E_0', E_1, and E_2 are the direct interband transitions, c_{11} and c_{12} the stiffness constants, and D_1^1 and D_3^3 the volume and shear deformation potentials, respectively. The stiffness constants are related to the compliance constants by $c_{11} - c_{12} = (S_{11} - S_{12})^{-1}$ and $c_{11} + 2c_{12} = (S_{11} + 2S_{12})^{-1}$.

[a]References [14-17];
[b]References [16-19];
[c]References [17, 20];
[d]This work: sample 1;
[e]This work: sample2;
[f]$E_2(X)$;
[g]$E_2(\Sigma)$.

The x dependence of the E_0' transition is small and a linear interpolation between the Si and Ge endpoints (see Tab. 1) can be used.

In recent experiments spectroscopic ellipsometry has been used to determine the shift in the E_1 gap [21-23] in strained $Si_{1-x-y}Ge_xC_y$ films. A linear decrease of E_1 with increasing effective Ge concentration was found [22], this in turn means that the incorporation of C leads to an increase in E_1.

In this paper, we will focus on the shift of the direct interband transitions in strained and relaxed $Si_{1-x-y}Ge_xC_y$ systems. We will show that the breakdown of continuum elasticity theory predicted by Theodorou *et al.* [7] and Demkov and Sankey [24] cannot be observed in our experiment. In the following section we will describe the evaluation of our data and discuss the theoretical background of biaxially stressed samples within the framework of elasticity theory and the influence of strain on the band structure. Finally we will show the spectra obtained from our samples and compare our results with the predictions.

THEORY

In strained layers we do not know the stress exerted on a layer, but we can determine the parallel and perpendicular components of the strain tensor from the lattice constants of the substrate and the free standing bulk alloy from elasticity theory [25, 26]

$$e_\perp = \frac{a_{Si}}{a_{xy}} - 1, \quad e_{||} = 2\frac{S_{12}}{S_{11}+S_{12}}e_\perp = -\frac{2\nu}{1-\nu}e_\perp, \tag{4}$$

where ν is Poisson's ratio. This results in a hydrostatic and shear strain given by

$$e_H = \frac{e_{||} + 2e_\perp}{3}, \quad e_S = \frac{e_{||} - e_\perp}{3}. \tag{5}$$

Shift and Splitting of the E_1 Gap

The E_1 and $E_1 + \Delta_1$ critical points in Si-like semiconductors originate from transitions along the Λ axis (or at the L point) of the Brillouin zone, that is parallel to [111]. These transitions were shown to be of excitonic nature [27] and an exchange interaction between the electron and hole can be observed. However, these interaction energies are very small, on the order of several meV ($\Delta E_{ex} \approx 4$ meV for the E_1 transition in $Si_{75}Ge_{25}$), and cannot be resolved in our experiments.

The spin-orbit splitting in Si ($\Delta_1^{Si} = 30$ meV) is too small to be observed. As we go to $Si_{1-x}Ge_x$ alloys with a considerable Ge content, we can resolve the E_1 and $E_1 + \Delta_1$ structure. We will use Eqs. (2)–(3) to calculate E_1 and $E_1 + \Delta_1$ for bulk $Si_{1-x}Ge_x$ and consider E_1^C linearly. It can be shown that the eigenvalues of the effective strain Hamiltonian are given by [28]

$$E_1 \quad = \quad E_1^0 + \frac{\Delta_1}{2} + \Delta E_H - \sqrt{\left(\frac{\Delta_1}{2}\right)^2 + (\Delta E_S)^2},$$

Figure 1: Limiting cases of the stress-induced splittings of the E_1 interband transitions for strained layers. The shown splitting corresponds to a biaxial compressive stress along [100] and [010]. Intensities were calculated from $\vec{k} \cdot \vec{p}$ perturbation theory starting from the bands at Γ. (a) Small shear aproximation and (b) large shear approximation.

$$E_1 + \Delta_1 \quad = \quad (E_1 + \Delta_1)^0 - \frac{\Delta_1}{2} + \Delta E_H + \sqrt{\left(\frac{\Delta_1}{2}\right)^2 + (\Delta E_S)^2}. \tag{6}$$

This splitting is shown in Fig. 1(a) for a biaxially compressed layer. Spin-orbit interaction splits the degenerate Λ_3 valence band into a doubly degenerate Λ_6 band and a $\Lambda_{4,5}$ doublet. Compressive biaxial stress has two effects on the band structure. Shear shift lowers the energy of E_1 and gives a blueshift in $E_1 + \Delta_1$ whereas hydrostatic strain increases the energy of both transitions. Therefore the shear and hydrostatic effects counteract each other for the E_1 transition and the shift is maximized for $E_1 + \Delta_1$. Biaxial stress influences E_1 much less than $E_1 + \Delta_1$. This can also be seen from Eq. (6).

The terms ΔE_H, ΔE_S are related to the strain tensor defined in the last section. Hydrostatic shift resulting from biaxial stress is represented by

$$\Delta E_H = 2\ \frac{D_1^1}{\sqrt{3}}\ (S_{11} + 2S_{12})X = \sqrt{3}\ D_1^1\ e_H. \tag{7}$$

This is twice the shift obtained for the uniaxial stress geometry for an applied stress X. The splitting due to the shear component of the strain is

$$\Delta E_S = \sqrt{\frac{2}{3}}\ D_3^3\ (S_{12} - S_{11})X = \sqrt{6}\ D_3^3\ e_S. \tag{8}$$

D_1^1 and D_3^3 are the volume and shear deformation potentials, respectively. Since values for Si and Ge are similar we will always take linear interpolations between Si and Ge to get the average deformation potentials and elastic constants.

In the large shear approximation (for small Δ_1) the spin-orbit term in Eq. (6) is neglected and we have two shear split transitions

$$E_a = E_1 + \Delta E_H + \Delta E_S, \quad E_b = E_1 + \Delta E_H - \Delta E_S \tag{9}$$

with relative intensities $\{E_a : E_b = 1 : 3\}$ [29], i.e. E_b dominates the spectrum (Fig. 1). For uniaxial stress a shift of E_1 with increasing stress was observed in Si [14]. In the case of biaxial stress, the shear split changes sign and we observe a transition for which hydrostatic and shear shift counteract each other and the net shift is minimized. For comparison the different splittings for the large and small shear approximation are shown together in Fig. 1. This result was confirmed experimentally by ellipsometric investigation of strained

Figure 2: Critical thickness for the growth of $Si_{1-x-y}Ge_xC_y$ layers on Si. The thick solid line represents $h_c = \infty$ since there is no net strain for $x = 8.087y$. The thin lines designate h_c = 4000, 2000, 1000, 500, 250 Å, respectively, decreasing from the center towards higher Ge or C contents.

$Si_{1-y}C_y$ alloys [10,25,26,30,31] where the large shear approximation is in good agreement with the spectra. It was found that hydrostatic and shear shift cancel ($\Delta E_H - \Delta E_S$ = -3 meV for $Si_{98.6}C_{1.4}$) and the net effect was an alloy shift of E_1 (75 meV for y=1.4%) [25,26,31]. The small shear approximation has been used by Pickering *et al.* [13] to explain shifts for a $Si_{78}Ge_{22}$ strained sample. Again the agreement between theory and experimental data was good.

E_0' and E_2 Transitions under Stress

Although it is commonly believed that the E_0' gap occurs at the Γ point, there is some controversy about the origin of this transition [15,29,32]. Ferrieu *et al.* [2] showed that E_0' follows a linear approximation over the $0 \leq x \leq 0.2$ range of composition for strained $Si_{1-x}Ge_x$. The composition dependence was found to be dE_0'/dx = -0.1 eV. In $Si_{1-y}C_y$, E_0' was found to vary linearly with y [30] or even to be constant [25,26]. Predictions are not reliable and further theoretical investigations are necessary.

In Si rich alloys we can resolve the two E_2 critical points which occur at the Σ and X points of the Brillouin zone [15]. These two points will merge into a single point as we increase the Ge content [19]. The E_2 transitions of Si and Ge are at about 4.3 eV. We know from $Si_{1-y}C_y$ strained layers that there is a shift in E_2 due to stress induced by lattice misfit between substrate and layer. Lange *et al.* [31] and Osten *et al.* [22] measured a decrease in $E_2(X)$ of -31 meV/1%[C] for $Si_{1-y}C_y$ alloys with a carbon content up to 1.4%. Investigations of the behavior of E_2 in Si-Ge-C films under biaxial stress have not been made.

Critical Thickness

The misfit between substrate and film is accommodated by a combination of uniform elastic strain and misfit dislocations. There is a critical thickness up to which all of the misfit is accommodated elastically [33,34]. In films above the critical thickness dislocations distort the lattice symmetry. In theoretical works on stacking faults [35,36] electronic defect states within the energy gap were found. This results in an inhomogeneous broadening and lower amplitudes of electronic transitions. The critical thickness h_c calculated by People and Bean [37] is

$$h_c \simeq \frac{1}{16\pi\sqrt{2}} \frac{1-\nu}{1+\nu} \frac{b^2}{a_{xy}} \frac{1}{e_\perp^2} \ln\left(\frac{h_c}{b}\right). \tag{10}$$

a_{xy} is the equilibrium bulk lattice constant of the alloy given by Eq. (1), b the Burger's vector ($b \approx a_{xy}/\sqrt{2}$), $e_\perp$ the stress in the growth plane, and ν the Poisson ratio. For strained Si-Ge layers h_c has been determined by energy balance calculations and found to be in good agreement with experiments [37]. Eq. (10) can be solved numerically. Fig. 2 shows the dependence of the critical thickness on the Ge and C content. The thick, solid line represents $h_c = \infty$, since for $x = 8.087y$ there is no net strain. The thin lines are h_c = 4000, 2000, 1000, 500, 250 Å, respectively. For comparison, our samples are also shown. For $h > h_c$, with h being the layer thickness, we can estimate the fraction χ of the misfit that is accommodated elastically by [34]

$$\chi = \frac{1+\ln(h/b)}{1+\ln(h_c/b)} \frac{h_c}{h} \tag{11}$$

with the remainder taken up by misfit dislocations. h_c and χ are given together with the specifications of the samples in Tab. 2.

Sample	x (%)	y (%)	Si cap (Å)	Si-Ge-C, h (Å)	h_c (Å)	χ (%)
1	25	0	1000	600	1130	100
2	30	0	100	2000	729	42
3	25	0.9	20	3000	2548	87
4	18	2	0	1000	420101	100
5	48	5	0	1000	18035	100

Table 2: $Si_{1-x-y}Ge_xC_y$ samples, their composition, layer thickness h, and critical thickness h_c. χ is the fraction of the misfit that is accommodated elastically, the remainder $(1-\chi)$ is taken up by misfit dislocations.

EXPERIMENTAL PROCEDURE AND DATA ANALYSIS

The samples discussed here were grown by MBE on Si(001) substrates at low temperatures so the C atoms are on lattice sites [38]. The series consists of five $Si_{1-x-y}Ge_xC_y$ samples with $0 \leq x \leq 48\%$ and $0 \leq y \leq 5\%$. Three of the samples have Si caps from 20 Å to 1000 Å. The values for x and y we give in Tab. 2 are nominal values determined by Rutherford backscattering (RBS), secondary-ion mass spectroscopy (SIMS), and x-ray diffraction (XRD) using Vegard's law, Eq. (1). Samples 1 and 2 are Si capped $Si_{1-x}Ge_x$ samples, one is a rather thin, strained layer and the other sample is a thick, partially relaxed film. There is a third sample with nearly the same Ge content but 0.9% C. Samples 4 and 5 are samples with high Ge and C contents. Sample 5 was grown at higher temperature so that only about 20% of the C is on lattice sites. XRD confirmed that there is only little net strain in samples 4 and 5, i.e., the strains from Ge and C are equal and opposite in sign.

To measure the pseudodielectric function $\langle\epsilon\rangle = \epsilon_1 + i\epsilon_2$ of the sample we used a rotating analyser ellipsometer (RAE) [39]. The measurements were taken at room temperature from 1.6 to 5.4 eV with a step size of 0.01 eV at an angle of incidence of 70°. In order to enhance the structure of the spectra the second derivative of ϵ with respect to energy is calculated. The critical point parameters were obtained by a least-squares fit to the second derivative of excitonic and two-dimensional (2D) one-electron CP line shapes [40]

$$\epsilon(E) = \begin{cases} C - A\ (E - E_{CP} - i\Gamma)^{-1}\ e^{i\Phi} & \text{excitonic} \\ C - A\ \ln(E - E_{CP} - i\Gamma)\ e^{i\Phi} & \text{2D.} \end{cases} \tag{12}$$

The procedure allows us to fit the real and imaginary parts simultaneously. The fit parameters are the amplitude A, phase angle Φ, critical point energy E_{CP}, and the line broadening Γ. For all samples a fit of E_1 and $E_1 + \Delta_1$ of the $Si_{1-x-y}Ge_xC_y$ layer to an excitonic line shape gave the best results. It was observed that in most cases the phase angle was close to that obtained for bulk Si. In alloys with about 25% Ge and only little carbon ($\leq 2\%$) we get an overlap of $E_1 + \Delta_1$ and E_0' transitions in $Si_{1-x-y}Ge_xC_y$. Instead of fitting two CP that are seperated by less than a typical line width (50-150 meV) we compensated for this effect by varying the phase angle to allow a mixture of excitonic and 2D lineshape and regard this point as a superposition. This necessarily leads to a considerably larger line width for that structure. Samples 1 and 2 have a Si cap and the CP's of the cap must also be considered. Here we took an excitonic line shape for E_1 and E_0' is represented by a 2D CP. The CP's in a 20 Å Si top on sample 3 cannot be detected. The E_2 features are described by 2D line shapes throughout the whole composition range.

RESULTS AND DISCUSSION

E_0', E_1 and $E_1 + \Delta_1$

We measured and analyzed the dielectric function of the samples described in the previous section. The results are shown in Tab. 1, 3 and 4. To calculate the theoretical values we used linear interpolations between the elastic constants and deformation potentials given in Tab. 1 and elasticity theory which was described earlier in this paper.

In the spectrum of sample 1 [Fig. 3(a)] four critical points were fitted in the 2.5-3.7 eV region. Data were obtained for E_1, $E_1 + \Delta_1$ of Si-Ge and E_0', E_1 of the Si cap. The data obtained for Si are in agreement

Figure 3: Second derivative of the dielectric function ϵ. Circles ($\bullet$) and triangles ($\triangle$) are the measured real and imaginary part of ϵ and solid and dashed lines are the best fits to an analytical line shape, respectively. (a) sample 1: $Si_{75}Ge_{25}$, (b) sample 2: $Si_{70}Ge_{30}$, (c) sample 4: $Si_{80}Ge_{18}C_2$, and (d) sample 3: $Si_{74.1}Ge_{25}C_{0.9}$.

with those for bulk Si (Tab. 1). Fig. 3(a) shows the second derivative of the spectrum of sample 1. Below the lowest direct gap the penetration depth of light increases rapidly from about 9 nm at 3.5 eV to nearly 2 μm at 2.5 eV. Therefore it is not surprising that we observe a strong peak from the $Si_{75}Ge_{25}$ layer although there is a 1000 Å Si cap on top. E_1 deviates 63 meV from theory. This may be due to interference effects below E_1 which make it difficult to determine the onset of E_1 [41]. $E_1 + \Delta_1$ agrees with predictions from elasticity theory. In alloys with about 25% Ge $E_1 + \Delta_1$ and E_0' are in general degenerate and can only be fitted as a single point. In this case we can resolve two points. However, we have to consider a contribution of E_0' from the Si-Ge layer to the same point originating from the Si cap. The E_0' structure may be a superposition of E_0' from $Si_{75}Ge_{25}$ and Si. We account for this by varying the phase angle for this CP. By doing this we get good agreement between our experiment and earlier results from bulk Si [15].

Sample 2 is a 2000 Å layer of $Si_{70}Ge_{30}$ with a 100 Å Si cap. Only E_1 of Si-Ge could be fitted, due to the low amplitude of the signal from the Si-Ge film [Fig. 3(b)]. The second derivative shows a weak structure at 2.910 eV which is attributed to E_1 of $Si_{70}Ge_{30}$ although theory predicts 3.007 eV for this CP. The spectrum is dominated by the E_1 peak of Si. E_1, E_0' of Si were fit and agree well with data obtained from bulk Si (see Tab. 1). It was found that the Si-Ge CP's have an amplitude that is reduced by a factor of 7 compared to sample 1 as can be seen in Fig. 3(a) and (b). This is due to relaxations and dislocations in the sample (58% of the strain is accommodated by dislocations) which lead to a weaker and inhomogeneously broadened peak [35,36].

In sample 1 the Si-Ge layer is 600 Å thick, well below the critical thickness which is 1129 Å for this alloy (see Fig.2 and Tab. 2) . This leads to a large signal from the Si-Ge film. Sample 2 is a 2000 Å layer with weak and broad Si-Ge transitions. The critical thickness for this composition is 729 Å implying that

Sample	Theory								Experiment	
	e_H (%)	e_S (%)	ΔE_H (meV)	ΔE_S (meV)	ΔE_A (meV)	Δ_1 (meV)	E_1 (eV)	$E_1+\Delta_1$ (eV)	E_1 (eV)	$E_1+\Delta_1$ (eV)
1	-0.43	0.62	70	71	-351	89	3.076	3.243	3.139	3.252
2	-0.52	0.74	84	86	-419	98	3.011	3.209	2.910	–
3	-0.31	0.44	50	50	-312	88	3.112	3.245	2.997	3.306
4	-0.03	0.05	5	5	-168	73	3.232	3.306	3.311	–
5	-0.13	0.19	21	23	-420	123	2.993	3.125	3.140	–

Table 3: Results for the E_1 and $E_1+\Delta_1$ transitions compared with theory. e_H, e_S are the hydrostatic and shear strain, ΔE_H, ΔE_S are the hydrostatic and shear shifts, respectively, ΔE_A is the alloy shift, and Δ_1 the spin-orbit splitting.

42% of the misfit is compensated elastically and the remaining 58% are accommodated by dislocations. For samples 1 and 2, the fit values for the Si critical points agree with those obtained for bulk Si (see Tab. 1). The amplitudes of those points are high and the line width and phase angle are the same as for Si. This indicates Si caps with very high crystalline quality, which is surprising since in sample 2 the SiGe layer underneath is heavily dislocated. The spectrum in Fig. 3(b) shows the dominant Si structure of the Si cap and only little influence from the Si-Ge layer.

Fig. 3(d) is a scan of sample 3 which has a similar composition as samples 1 and 2. However, the 3000 Å film is stabilized by the incorporation of 0.9% C which compensates for the stress of 7.27% Ge. Therefore the critical thickness increased to 2548 Å. The thin Si cap is invisible since the structures from the Si-Ge film are strong. This shows that the critical thickness of a film can be increased considerably by substitution of small amounts of C in Si-Ge. For sample 3 E_1 and a structure at 3.306 eV could be fitted. The latter is a superposition of $E_1+\Delta_1$ and E_0'. Possible contributions from the Si cap can not be excluded and a comparison with theory is difficult. With three critical points this part of the spectrum is overdetermined and the data are not reliable. Therefore only two points are fitted to the experimental curves. The measured E_1 is 115 meV lower than predicted by theory and the peak at 3.306 eV is an average of E_0' which is expected at 3.36 eV and $E_1+\Delta_1$ which is expected at 3.245 eV.

Figs. 3(c) and 4 show the dielectric function of two strain free samples, i.e. samples 4 and 5. The line width in those samples is increased to 200 - 250 meV and it is no longer possible to resolve E_1–$(E_1+\Delta_1)$ or even the E_0' transition, which is believed to depend only weakly on composition [2]. In the spectra of sample 4 we see a somewhat broadened peak at a position in between those points and again the predictions from elasticity theory agree with the observed shifts. Sample 5 has many dislocation due to the large amount of carbon in this alloy. Furthermore sample 5 was grown at a higher temperature than samples 1–4. Only about 20% of the C atoms are on substitutional lattice sites and the crystal structure is heavily distorted. The spectrum of sample 5 shows Ge E_1 and $E_1+\Delta_1$ transitions which are not expected in an alloy. This indicates Ge clustering in this sample. Two peaks at 2.113 eV and 2.326 eV were fitted and assigned to E_1 and $E_1+\Delta_1$ of bulk Ge. The spin-orbit splitting is found to be 212 meV and compares well with previous experiments [19]. The dashed arrow in Fig. 4 indicates a weak structure at 3.14 eV. The origin of this peak (that has an amplitude just above the noise level) is not clear. It could originate from clusters of unknown compositions that were favored under the changed growth conditions. Sample 5 can be regarded as an amorhpous film with considerable Ge clustering rather than an alloy.

E_2 Region

Even in samples with many dislocations the E_2 transitions are expected to be relatively strong compared to the otherwise dominant E_1 structure. This is due to the origin of E_2 CP's which extends over a large part of the Brillouin zone predominantly in the $X-\Sigma$ plane and distortions do not affect these peaks as much as the E_1 transition which occurs in a narrow part of the BZ.

Two of the samples investigated have Si caps which can be fit in the spectra. Since the penetration depth in Si drops to below 100 Å above the E_1 gap, which is between 2.9 eV and 3.5 eV for our samples, the E_2 transitions of the covered Si-Ge film are not visible with ellipsometry. Therefore the spectra of samples

Figure 4: (a) Dielectric function of sample 5: $Si_{47}Ge_{48}C_5$. Second derivatives of the (b) real and (c) imaginary part of ϵ are shown with corresponding least square fit results. The dashed arrow in (b) indicates the position of a weak Si-Ge-C structure that could be fitted. The dominant features in this sprectrum are the E_1 and $E_1 + \Delta_1$ transitions of Ge.

1 and 2 exhibit Si characteristics in the 4–5 eV energy range. We fitted $E_2(X)$ and $E_2(\Sigma)$ of the Si cap. For both transitions a 2D line shape yields the best fit. The obtained $E_2(X)$ and $E_2(\Sigma)$ energies are in satisfactory agreement with those measured in bulk Si (Tab. 4). Since the thickness of the Si cap on sample 3 is less than the penetration depth of the light, the measured E_2 is a mixture with contributions from both the film as well as the cap. For samples 3 and 4, the E_2 transitions follow the predictions which are a linear interpolation between $E_2(X)$ in Si, which is the stronger of the two Si transitions, and Ge (Tab. 4). Spectra of sample 5 show a weak and broad structure at 4.391 eV. This peak is close to the transition

Sample	Experiment E_2 (eV)		Theory E_2 (eV)	
1	4.275	4.542	4.270[a]	4.492[b]
2	4.279	4.506	4.270[a]	4.492[b]
3	4.299		4.295[c]	
4	4.273		4.288[c]	
5	4.391		4.368[d]	

Table 4: Energies and origins of the observed E_2 transitions. For Si-Ge-C we used a linear interpolation between Si and Ge, neglecting C.

[a]Si, $E_2(X)$
[b]Si, $E_2(\Sigma)$
[c]Si-Ge-C
[d]Ge

energy in bulk Ge but an assignment of this point to a Ge transition difficult due to the low amplitude which leads to a large error in the determination of the energy. But since we already know that sample 5 shows Ge transitions at lower energies it can be assumed that this point also originates from Ge clusters. Overall no stress dependence of E_2 can be found in our experiments although a shift was expected from previous experiments on Si-C alloys [31, 22, 23]. Further investigation of this part of the spectrum is necessary to completely understand the behavior of transitions in the X–Σ region of the BZ in Si-like alloys under biaxial stress.

CONCLUSION

Continuing previous works on the effects of strain on the band structure of group IV semiconductor alloys [25, 26, 31, 41] we have determined the hydrostatic and shear shifts in biaxially stressed Si-Ge-C films using rotating-analyser ellipsometry. Starting from the stress tensor for a biaxial stress along [010] and [100], we derived expressions for the shifts in E_1 and $E_1 + \Delta_1$ of zinc-blende type crystals from elasticity theory based on the well established concept of deformation potentials. This theory was applied to the ternary Si-Ge-C alloy system and satisfactory agreement between the predicted and observed shifts was found.

We investigated five $Si_{1-x-y}Ge_xC_y$ samples in the range $0 \leq x \leq 48\%$ and $0 \leq y \leq 5\%$ grown by MBE on Si(001). Two of the samples were $Si_{1-x}Ge_x$ films with a Si cap. Here we recovered the E_0', E_1 Si critical points at energies which compare well with those of bulk Si. Nevertheless, structures originating from the buried film were detected and compared with the results of elasticity theory. Sample 3 was a strained Si-Ge-C film with 25% Ge that was stabilized by the incorporation of 0.9% C. Although the layer is beyond the critical thickness, we could clearly observe the E_1 and $E_1 + \Delta_1$ transitions of the strained film. Samples 4 and 5 were assumed to be strain-free samples with high C concentrations. This was confirmed for sample 4 although a broadening of the CP's due to dislocations and distortions of the crystal lattice near substitutional C atoms made it impossible to fit more than one critical point to the observed structure between 2.5 and 3.5 eV which is believed to be dominated by the E_1 transition. Sample 5 showed Ge E_1 and $E_1 + \Delta_1$ points which originate from Ge clusters in the film. One critical point at a position in between E_1, $E_1 + \Delta_1$, and E_0' could be fit. In every case, elasticity theory can account for the observed shifts of E_1 and $E_1 + \Delta_1$. No stress dependence of E_2 could be found and a linear interpolation between the Si and Ge endpoints is in good agreement with the experimental data. Further investigations are necessary to understand the behavior of E_0' and E_2 in Si-Ge-C strained films. Current experiments are devoted to this topic.

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